

chain nodes :

12 13 20 21 22 23 24 31 32 33

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18 19 25 26 27 28
29 30

chain bonds :

7-21 8-12 9-20 10-13 11-14 20-22 21-31 22-23 22-24 23-25 31-32
31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-11 7-8 8-9 9-10 10-11 14-15
14-19 15-16 16-17 17-18 18-19 25-26 25-30 26-27 27-28 28-29
29-30

exact/norm bonds :

5-7 6-11 7-8 7-21 8-9 8-12 9-10 9-20 10-11 10-13 11-14 20-22
22-23 22-24 23-25 31-32 31-33

exact bonds :

21-31

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19
25-26 25-30 26-27 27-28 28-29 29-30

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS
33:CLASS

09/980,987

=> d his

(FILE 'HOME' ENTERED AT 19:03:21 ON 31 JAN 2003)

FILE 'REGISTRY' ENTERED AT 19:03:26 ON 31 JAN 2003

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 14 S L2

L4 402 S L2 SSS FUL

FILE 'CAPLUS' ENTERED AT 19:05:48 ON 31 JAN 2003

L5 49 S L4

FILE 'REGISTRY' ENTERED AT 19:06:17 ON 31 JAN 2003

L6 STRUCTURE UPLOADED

L7 QUE L6

L8 9 S L7

L9 208 S L7 SUB=L4 FUL

FILE 'CAPLUS' ENTERED AT 19:06:57 ON 31 JAN 2003

L10 34 S L9

L11 ANALYZE L10 1- RN HIT : 247 TERMS

FILE 'REGISTRY' ENTERED AT 19:07:24 ON 31 JAN 2003

L12 1 S 151386-96-8/RN

L13 STRUCTURE UPLOADED

L14 QUE L13

L15 0 S L14 SUB=L4 SAM

L16 71 S L14 SUB=L4 FUL

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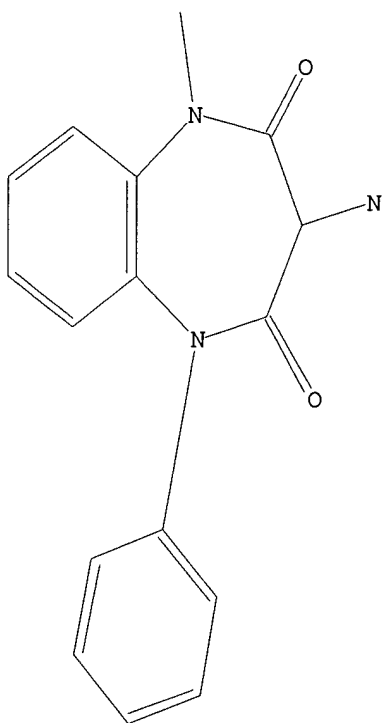
L17 9 S L16

=> d 12

L2 HAS NO ANSWERS

L1 STR

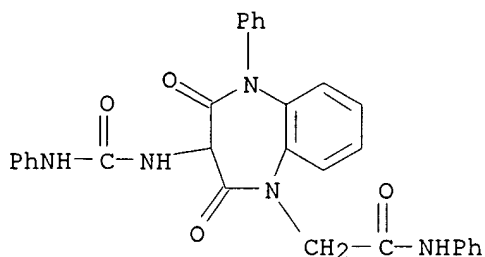
09/980,987



Structure attributes must be viewed using STN Express query preparation.
L2 QUE ABB=ON PLU=ON L1

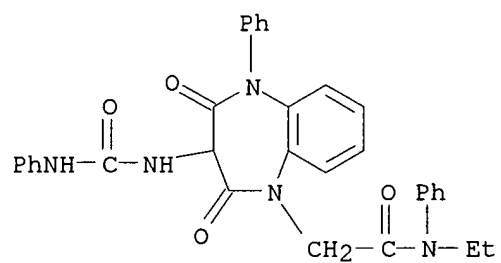
=> d bib abs hitstr 1-9

~~LN~~ 7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS
~~IN~~ 2001:168978 CAPLUS
 DN 134:335989
 TI Nonpeptide cholecystokinin-2 receptor agonists
 AU Kalindjian, S. Barret; Dunstone, David J.; Low, Caroline M. R.; Pether, Michael J.; Roberts, Sonia P.; Tozer, Matthew J.; Watt, Gillian F.; Shankley, Nigel P.
 CS James Black Foundation, London, SE24 9JE, UK
 SO Journal of Medicinal Chemistry (2001), 44(8), 1125-1133
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 AB In the course of structural explorations around a series of potent CCK2 receptor antagonists, it was noted that simple N-methylation of the indolic N-H in the parent mol. gave rise to behavior in vivo that was consistent with the compd. acting as an agonist. Exploration in vitro confirmed this property, and it was shown that the agonist action could be blocked by the ref. CCK2 receptor antagonist, L-365,260. Further examples of this type of modification were explored, and a common theme with regard to agonist behavior was uncovered. Some mol. modeling is also presented in an attempt to throw light on the nature of the ligand receptor interactions that may be giving rise to the differing properties of these, apparently, structurally similar mols.
 IT **173908-65-1P 173908-67-3P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (structure-activity relationship of nonpeptide cholecystokinin-2 receptor agonists)
 RN 173908-65-1 CAPLUS
 CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 173908-67-3 CAPLUS
 CN 1H-1,5-Benzodiazepine-1-acetamide, N-ethyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)

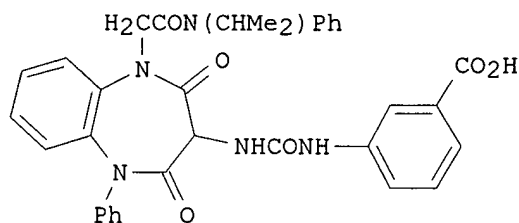
09/980,987



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS
 AN 2000:814470 CAPLUS
 DN 133:350255
 TI Preparation of 1,5-benzodiazepine derivatives as CCK-A receptor agonists
 IN Colclough, David; Hodgson, Anne; Szewczyk, Jerzy Ryszard
 PA Glaxo Group Ltd., UK
 SO PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000068209	A2	20001116	WO 2000-EP3982	20000504
	WO 2000068209	A3	20010301		
	W:		AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
	RW:		GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
	BR 2000010338	A	20020213	BR 2000-10338	20000504
	EP 1212305	A2	20020612	EP 2000-929488	20000504
	R:		AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL		
	JP 2002544200	T2	20021224	JP 2000-617189	20000504
	NO 2001005397	A	20011105	NO 2001-5397	20011105
PRAI	GB 1999-10366	A	19990506		
	GB 2000-8179	A	20000405		
	WO 2000-EP3982	W	20000504		
OS	MARPAT 133:350255				
GI					



AB An enantiomerically enriched 1,5-benzodiazepine compd. I is disclosed.
 Use of I for the treatment of CCK-A mediated diseases or conditions, such as obesity, is indicated.

IT **305366-98-7P 305366-99-8P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

09/980,987

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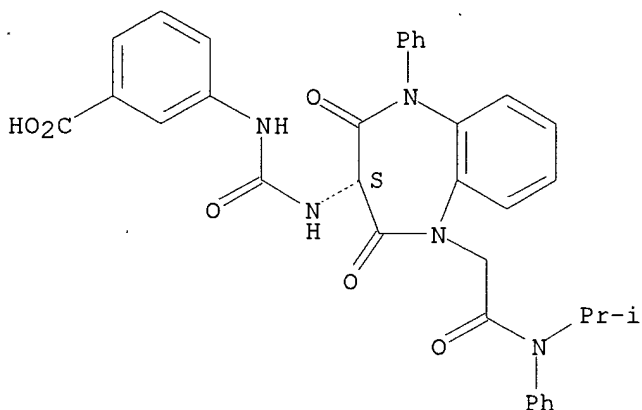


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RN 305366-98-7 CAPLUS

CN Benzoic acid, 3-[[[[(3S)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

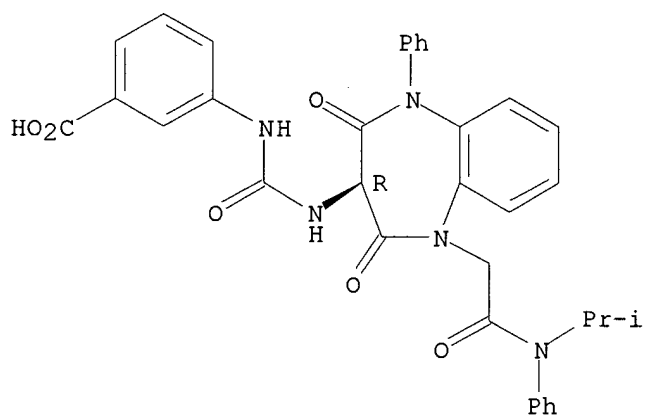
Absolute stereochemistry. Rotation (+).



RN 305366-99-8 CAPLUS

CN Benzocic acid, 3-[[[(3R)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 305366-94-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

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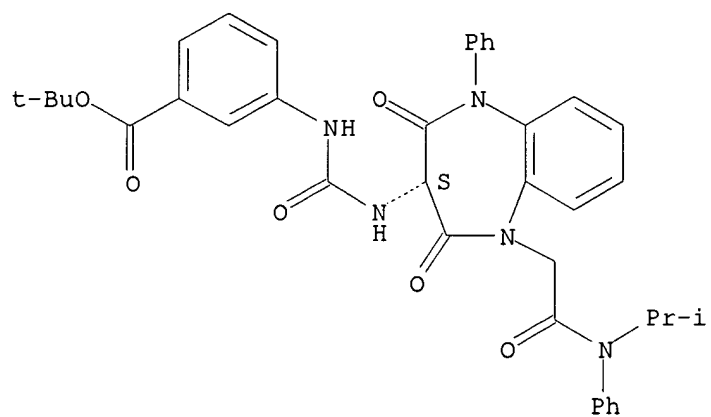


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RN 305366-94-3 CAPLUS

CN Benzoic acid, 3-[[[[(3S)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



~~LI~~ ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS

~~AN~~ 2000:391139 CAPLUS

DN 133:129526

TI Computer prediction of biological activity spectra for low-molecular peptides and peptidomimetics

AU Martynova, N. B.; Filimonov, D. A.; Poroikov, V. V.

CS Institute of Biomedical Chemistry, Russian Academy of Medical Sciences, Moscow, 119832, Russia

SO Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya) (2000), 26(5), 297-305

CODEN: RJBCEJ; ISSN: 1068-1620

PB MAIK Nauka/Interperiodica

DT Journal

LA English

AB The wide variety of the biol. effects of peptides and their high activity are the main reasons for the search for new basic drug structures among them. The most promising compds. can be selected using the PASS computer system (Prediction of Activity Spectra for Substances). This system was originally developed to predict the activities of low-mol. "drug-like" org. compds. Its predictive capacity is described here by the example of 134 peptides and peptidomimetics with nine known biol. activities. Its av. predictive power is shown to be approx. 97%. Such an accuracy demonstrates that computer prediction can be applied both to the evaluation of effects and mechanisms of action of endogenous and synthetic peptides and to the screening of new therapeutic agents among the most promising basic structures.

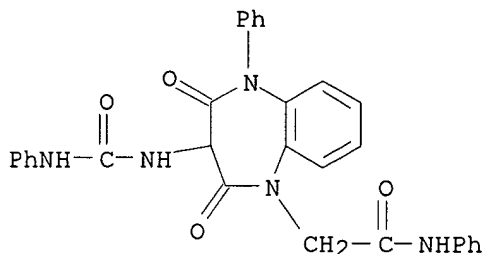
IT 173908-65-1 173908-66-2 173908-67-3
173908-68-4 173908-69-5 173908-70-8
173908-71-9 173908-72-0 173908-73-1
173908-75-3 173908-76-4 173908-77-5
173908-78-6 173908-79-7 173908-82-2
173908-83-3 173908-84-4 173908-85-5
173908-86-6 173908-87-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(cholecystokinin receptor agonist; computer prediction of biol. activity spectra for low-mol. peptides and peptidomimetics)

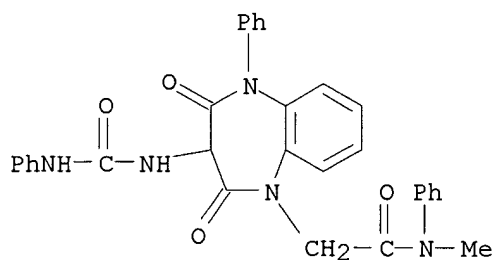
RN 173908-65-1 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



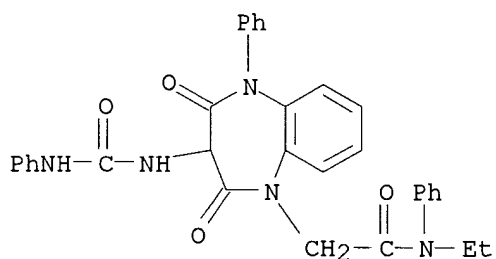
RN 173908-66-2 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



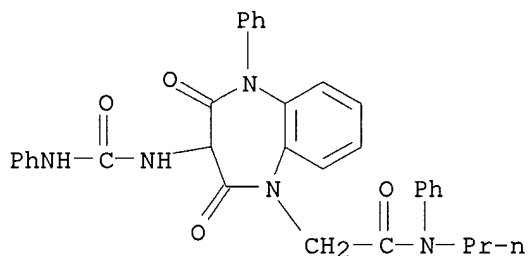
RN 173908-67-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-ethyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



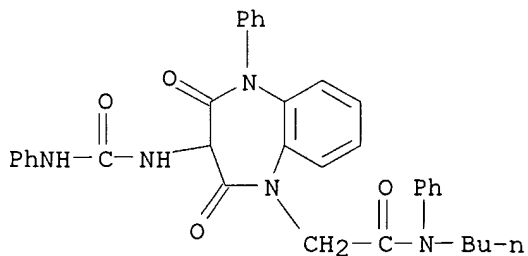
RN 173908-68-4 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]-N-propyl- (9CI) (CA INDEX NAME)



RN 173908-69-5 CAPLUS

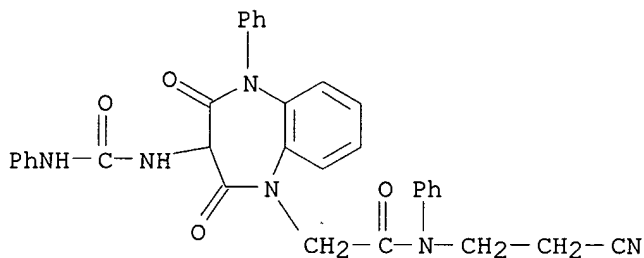
CN 1H-1,5-Benzodiazepine-1-acetamide, N-butyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



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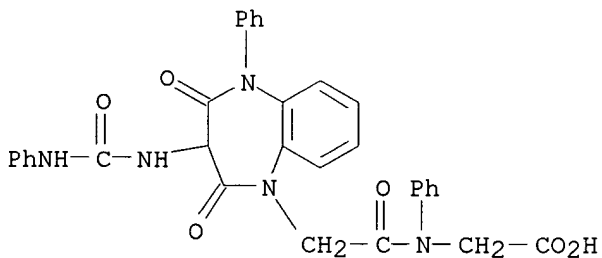
RN 173908-70-8 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-cyanoethyl)-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



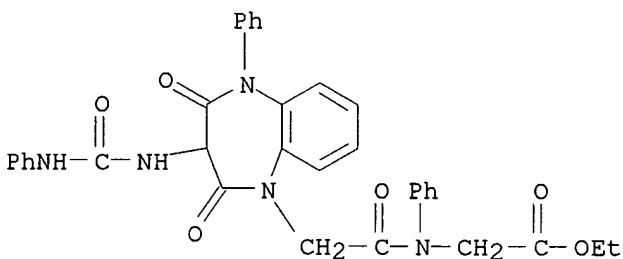
RN 173908-71-9 CAPLUS

CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)



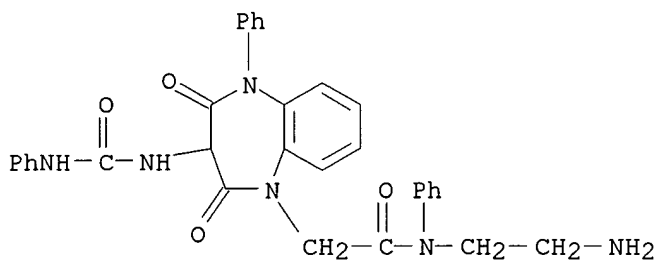
RN 173908-72-0 CAPLUS

CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



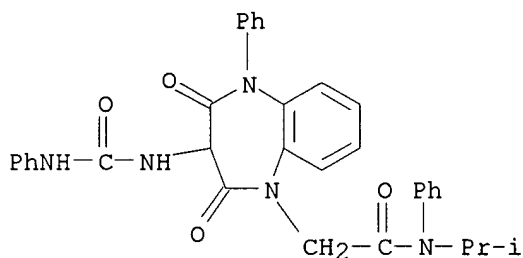
RN 173908-73-1 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-aminoethyl)-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



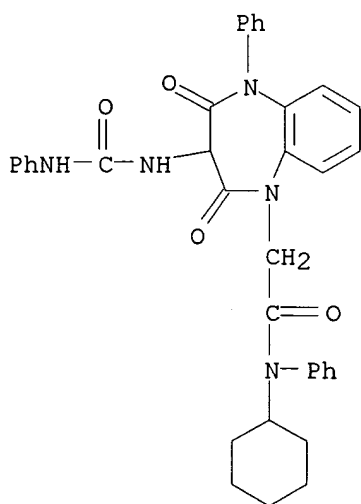
RN 173908-75-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



RN 173908-76-4 CAPLUS

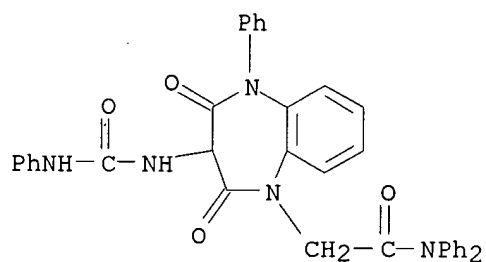
CN 1H-1,5-Benzodiazepine-1-acetamide, N-cyclohexyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



RN 173908-77-5 CAPLUS

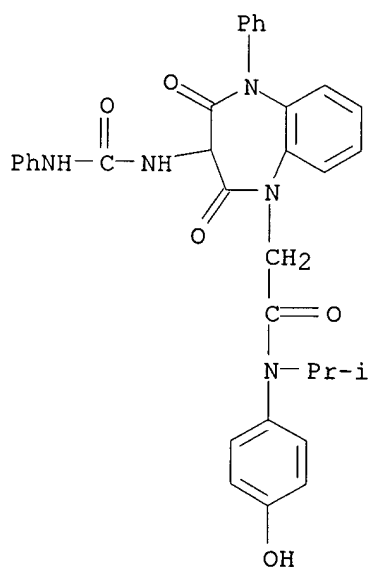
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,N,5-triphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)

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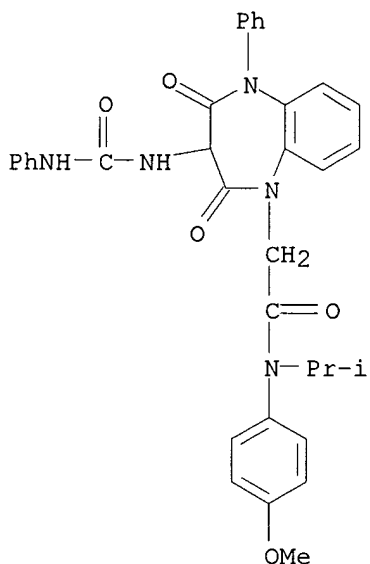
RN 173908-78-6 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-hydroxyphenyl)-
N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-
(9CI) (CA INDEX NAME)

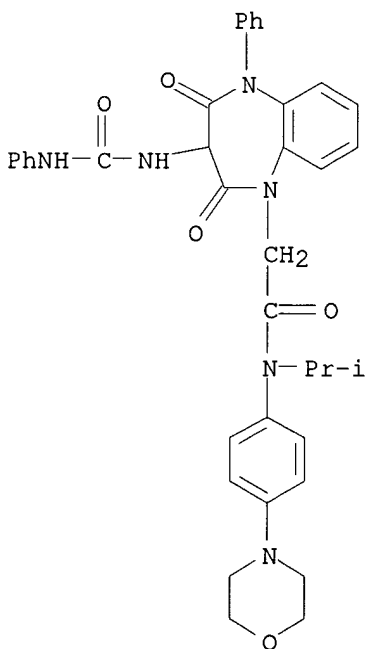


RN 173908-79-7 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-
N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-
(9CI) (CA INDEX NAME)

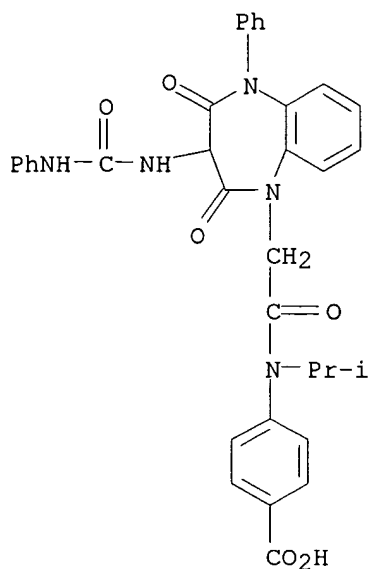


RN 173908-82-2 CAPLUS
 CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-N-[4-(4-morpholinyl)phenyl]-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



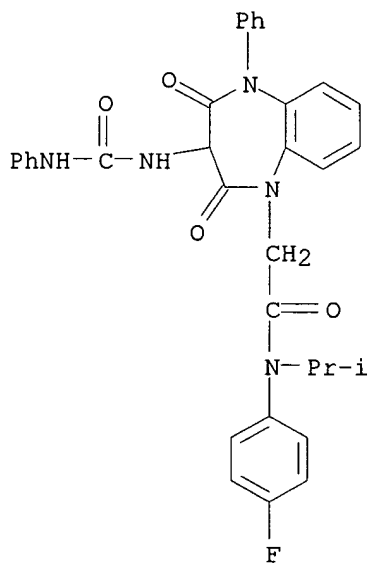
RN 173908-83-3 CAPLUS
 CN Benzoic acid, 4-[(1-methylethyl) [[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-yl] acetyl] amino]- (9CI) (CA INDEX NAME)

09/980,987



RN 173908-84-4 CAPLUS

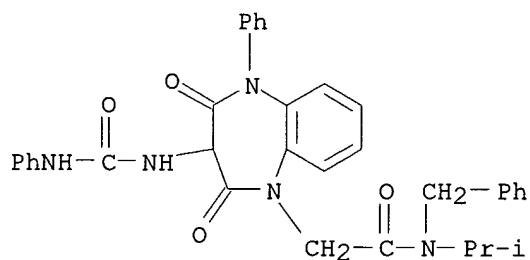
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(4-fluorophenyl)-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino] - (9CI)
(CA INDEX NAME)



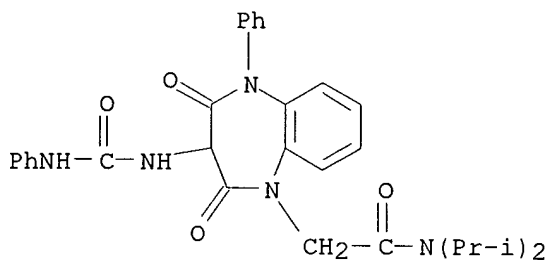
RN 173908-85-5 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino] -N-(phenylmethyl) - (9CI) (CA INDEX NAME)

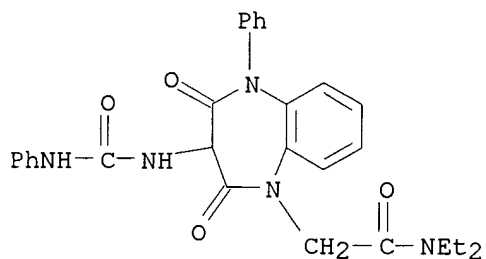
09/980,987



RN 173908-86-6 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N,N-bis(1-methylethyl)-2,4-dioxo-5-phenyl-3-[(phenylamino)carbonyl]amino]- (9CI)
(CA INDEX NAME)



RN 173908-87-7 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N,N-diethyl-2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~LI~~ ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS

~~AN~~ 1999:1261 CAPLUS

DN 130:163293

TI Structurally similar small molecule photoaffinity CCK-A agonists and antagonists as novel tools for directly probing 7TM receptor-ligand interactions

AU Darrow, James W.; Hadac, Elizabeth M.; Miller, Laurence J.; Sugg, Elizabeth E.

CS Neurogen Corporation, Branford, CT, 06405, USA

SO Bioorganic & Medicinal Chemistry Letters (1998), 8(22), 3127-3132

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB Incorporation of photolabile benzoyl (2a-d) or trifluoromethyl-3H-diazirine (3a-d) substituents into 1,5-benzodiazepine ligands did not significantly impair the rat CCK-A binding affinity of either agonists or antagonists. The modified agonist ligands also retained functional potency and efficacy in the rat amylase assay. Despite their strong structural similarity, the SAR of this limited set of compds. suggests that these small mol. antagonists and agonists might differ in their mode of binding to the CCK-A receptor. Preliminary affinity results show that representative agonists and antagonists from these series can be used to efficiently covalently label the CCK-A receptor.

IT 220493-38-9P 220493-39-0P 220493-40-3P

220493-41-4P 220493-42-5P 220493-43-6P

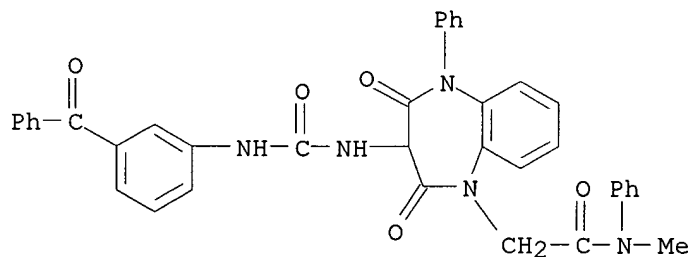
220493-44-7P 220493-45-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PNU (Preparation, unclassified); BIOL (Biological study); PREP (Preparation)

(affinity of, to bind CCK-A receptor,; incorporation of photolabile benzoyl or trifluoromethyl-3H-diazirine substituents into benzodiazepine ligands)

RN 220493-38-9 CAPLUS

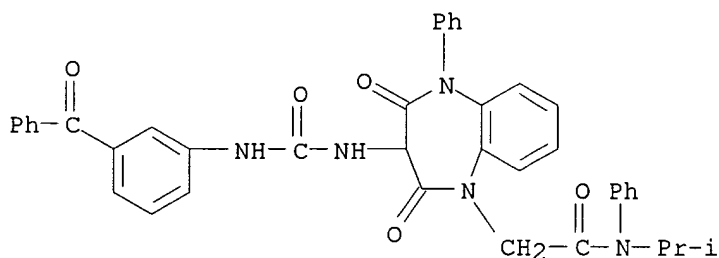
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



RN 220493-39-0 CAPLUS

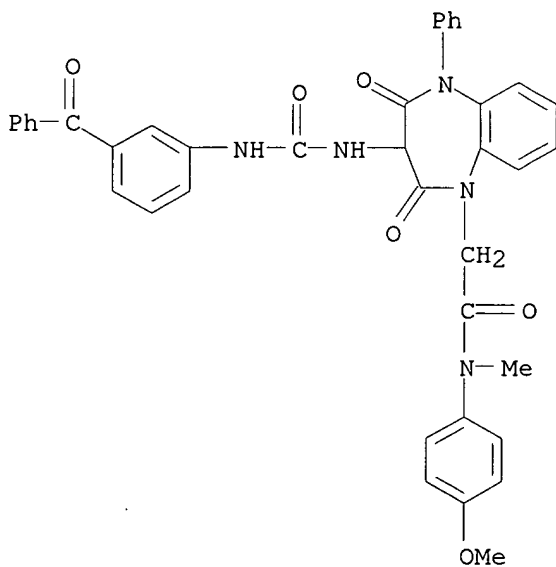
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)

09/980,987



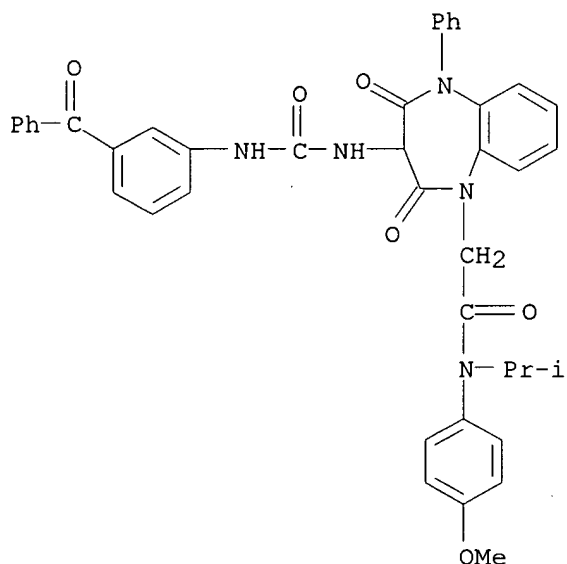
RN 220493-40-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-methyl-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



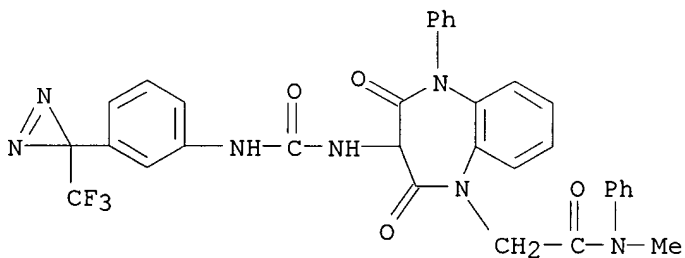
RN 220493-41-4 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-benzoylphenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



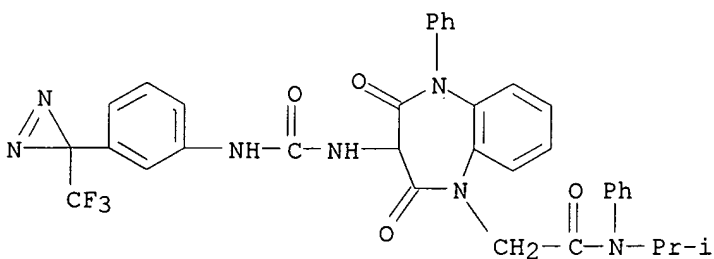
RN 220493-42-5 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl-3-[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 220493-43-6 CAPLUS

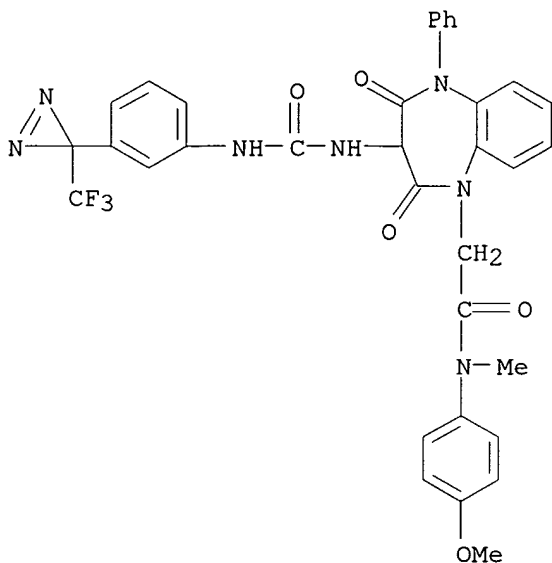
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 220493-44-7 CAPLUS

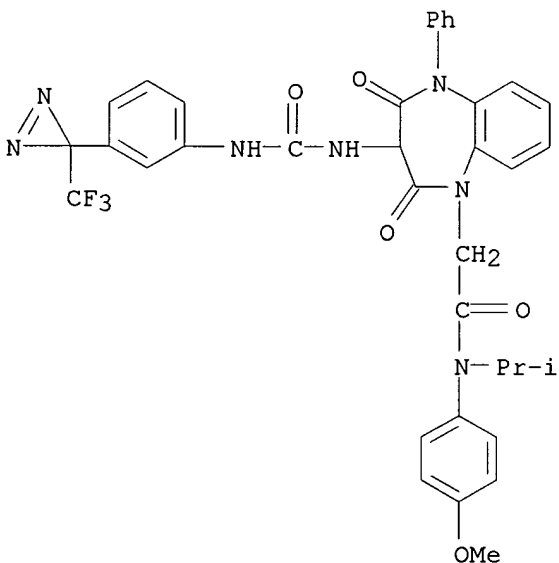
09/980,987

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-methyl-2,4-dioxo-5-phenyl-3-[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 220493-45-8 CAPLUS

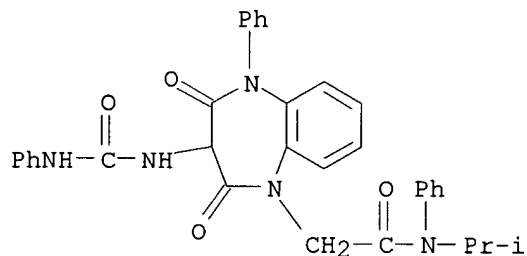
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



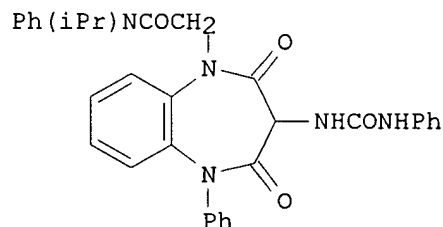
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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~~LN~~ 7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1997:188924 CAPLUS
~~DN~~ 126:271812
 TI Conversion of acyclic nonpeptide CCK antagonists into CCK agonists
 AU Hirst, Gavin C.; Queen, Kennedy L.; Sugg, Elizabeth E.; Willson, Timothy M.
 CS Department of Medicinal Chemistry, Glaxo Wellcome Research and Development, Research Triangle Park, NC, 27709, USA
 SO Bioorganic & Medicinal Chemistry Letters (1997), 7(5), 511-514
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier
 DT Journal
 LA English
 OS CASREACT 126:271812
 AB The CCK antagonists RP 69758 and (R)-lorglumide were converted into CCK agonists by the introduction of an N-isopropylanilide agonist "trigger". The common structural features of these ligands suggest that nonpeptide agonists and antagonists bind to a common site in the CCK receptor.
 IT **173908-75-3**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (conversion of acyclic nonpeptide cholecystokinin antagonists into cholecystokinin agonists by structural modification)
 RN 173908-75-3 CAPLUS
 CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)



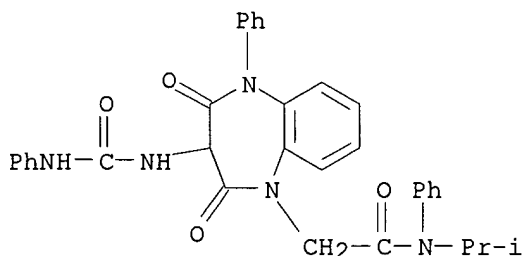
L17 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2003 ACS
 AN 1996:713053 CAPLUS
 DN 126:42245
 TI Discovery of 1,5-Benzodiazepines with Peripheral Cholecystokinin (CCK-A) Receptor Agonist Activity (II): Optimization of the C3 Amino Substituent
 AU Hirst, Gavin C.; Aquino, Christopher; Birkemo, Lawrence; Croom, Dallas K.; Dezube, Milana; Dougherty, Robert W., Jr.; Ervin, Gregory N.; Grizzle, Mary K.; Hanke, Brad; et al.
 CS Department of Medicinal Chemistry, Glaxo Wellcome Research and Development, Research Triangle Park, NC, 27709, USA
 SO Journal of Medicinal Chemistry (1996), 39(26), 5236-5245
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 GI



AB Analogs of the previously reported 1,5-benzodiazepine peripheral cholecystokinin (CCK-A) receptor agonist (I) were prepd. which explore substitution and/or replacement of the C-3 Ph urea moiety. Agonist efficacy on the isolated guinea pig gallbladder (GPGB) was retained with a variety of substituted ureas and amide analogs. Three compds. were identified which were orally active in the mouse gallbladder emptying assay (MGBE). The 2-indolamide and N-(carboxymethyl)-2-indolamide derivs. had improved affinity for the human CCK-A receptor but reduced agonist efficacy on the GPGB. Neither indolamide was orally active in a rat feeding assay. In contrast, the (3-carboxyphenyl)urea deriv. (GW7854) had moderately increased affinity for the human CCK-B receptor but was a potent full agonist on the GPGB and was orally active in both the MGBE and rat feeding assays. GW7854 was a full agonist (EC₅₀ = 60 nM) for calcium mobilization on CHO K1 cells expressing hCCK-A receptors and a potent antagonist of CCK-8 (pA₂ = 9.1) on CHO K1 cells expressing hCCK-B receptors. GW7854 is a potent mixed CCK-A agonist/CCK-B antagonist which is orally active in two in vivo models of CCK-A-mediated agonist activity.

IT **173908-75-3**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (prepn. and structure activity relations of 1,5-benzodiazepines as peripheral cholecystokinin (CCK-A) receptor agonists)

RN 173908-75-3 CAPLUS
 CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



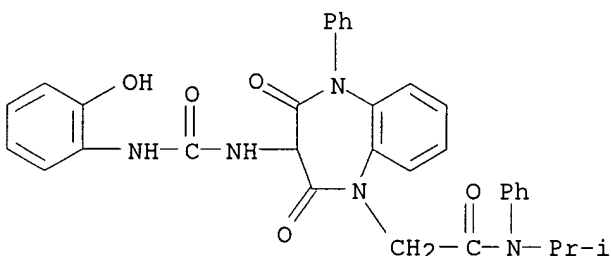
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 184944-97-6P 184944-98-7P 184944-99-8P
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 184945-03-7P 184945-04-8P 184945-05-9P
 184945-06-0P 184945-07-1P 184945-08-2P
 184945-09-3P 184945-10-6P 184945-11-7P
 184945-12-8P 184945-13-9P 184945-14-0P
 184945-15-1P 184945-16-2P 184945-30-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and structure activity relations of 1,5-benzodiazepines as peripheral cholecystokinin (CCK-A) receptor agonists)

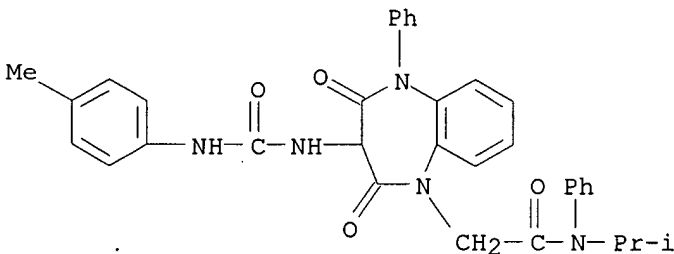
RN 184944-94-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(2-hydroxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



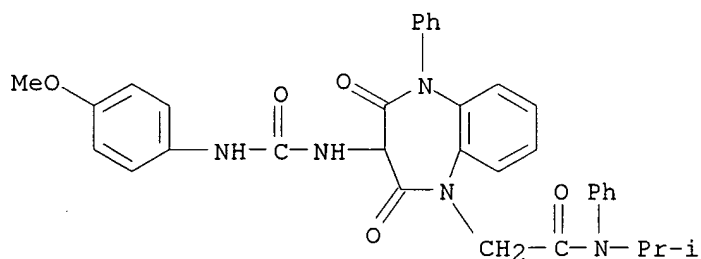
RN 184944-95-4 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(4-methylphenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



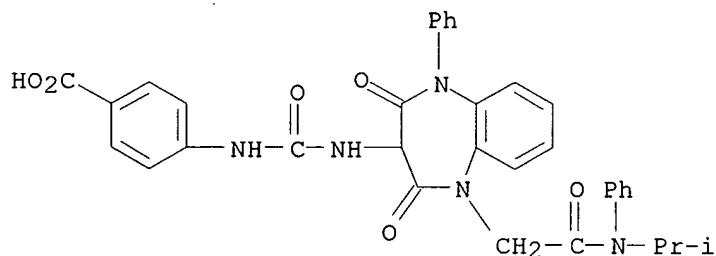
RN 184944-96-5 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(4-methoxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



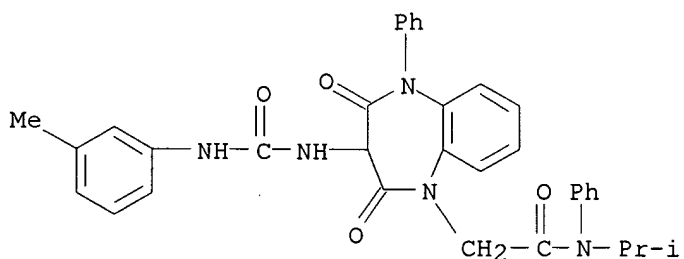
RN 184944-97-6 CAPLUS

CN Benzoic acid, 4-[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 184944-98-7 CAPLUS

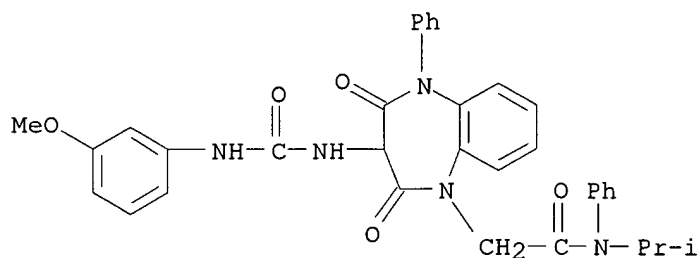
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(3-methylphenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



RN 184944-99-8 CAPLUS

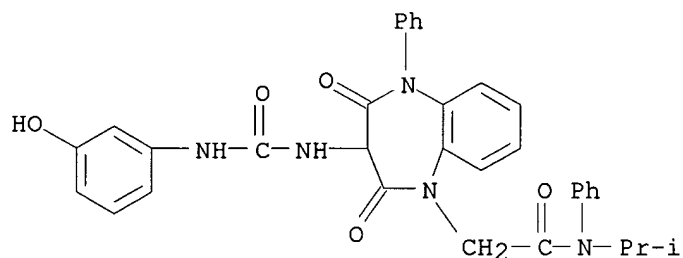
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(3-methoxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)

09/980,987



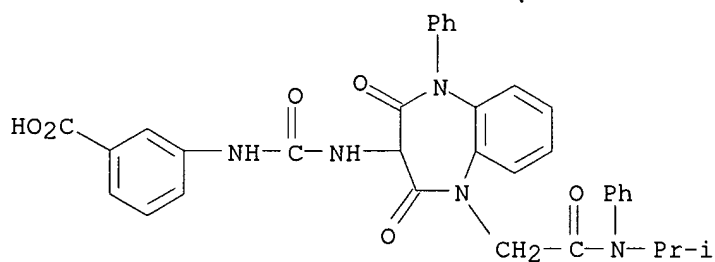
RN 184945-00-4 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(3-hydroxyphenyl)amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



RN 184945-01-5 CAPLUS

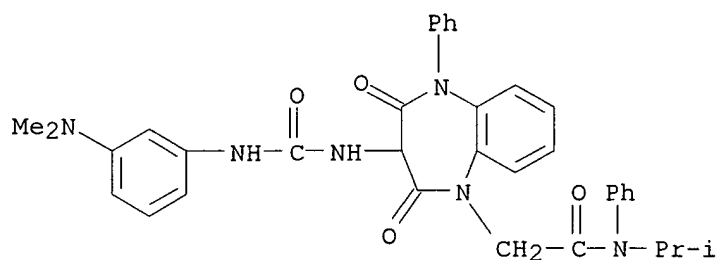
CN Benzoic acid, 3-[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 184945-02-6 CAPLUS

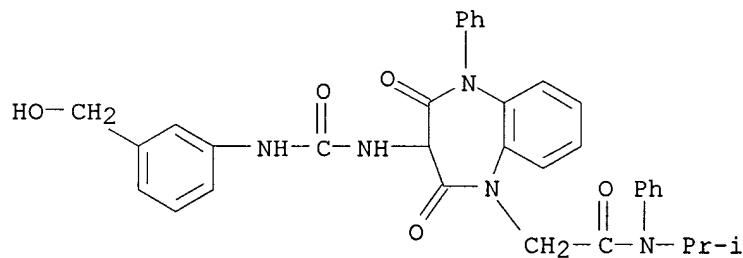
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[3-(dimethylamino)phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)

09/980,987



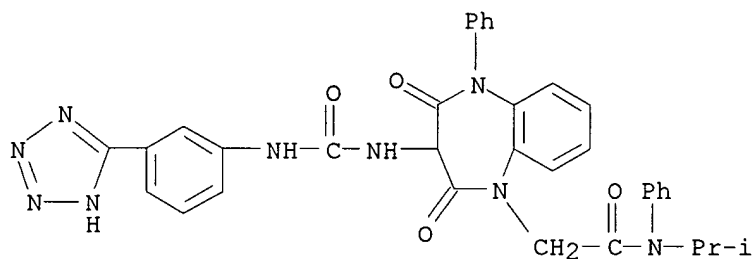
RN 184945-03-7 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[3-(hydroxymethyl)phenyl]amino]carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



RN 184945-04-8 CAPLUS

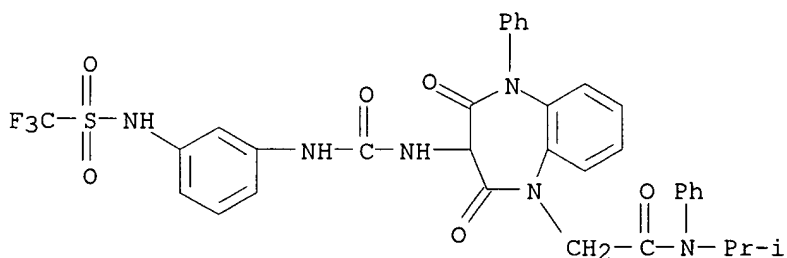
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[[3-(1H-tetrazol-5-yl)phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 184945-05-9 CAPLUS

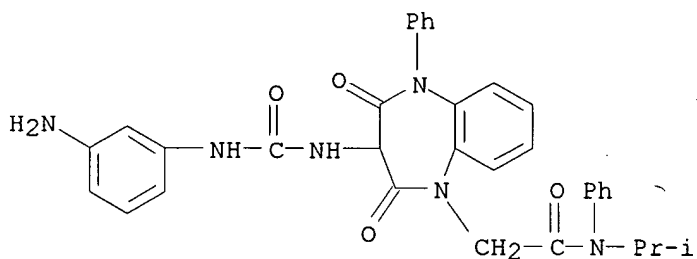
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[[3-[[[trifluoromethyl]sulfonyl]amino]phenyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

09/980,987



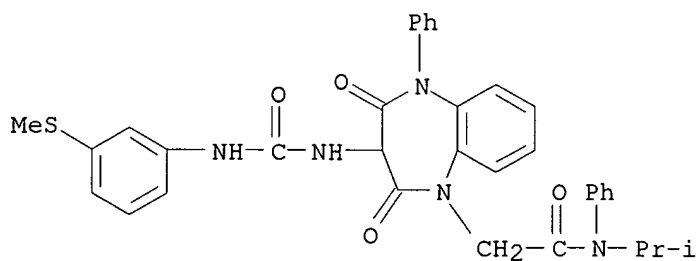
RN 184945-06-0 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-aminophenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



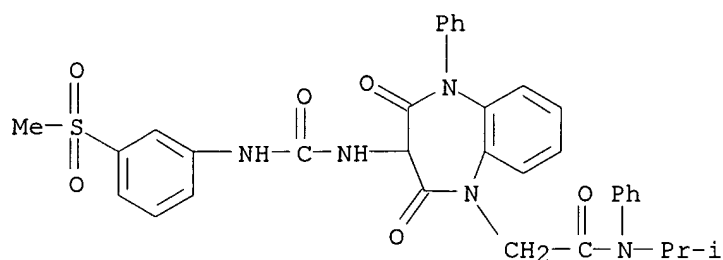
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CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(3-(methylthio)phenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



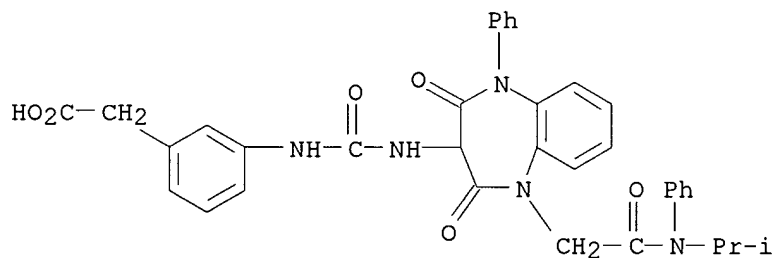
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CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[(3-(methylsulfonyl)phenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



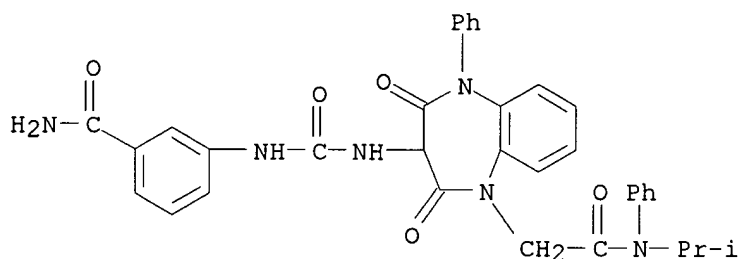
RN 184945-09-3 CAPLUS

CN Benzeneacetic acid, 3-[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



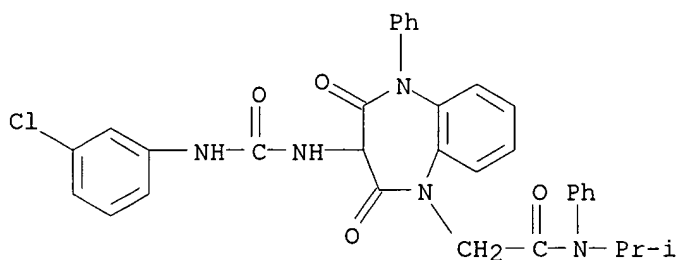
RN 184945-10-6 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[3-(aminocarbonyl)phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



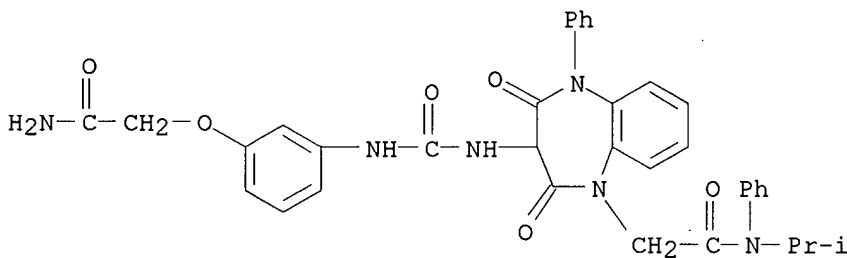
RN 184945-11-7 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[3-(chlorophenyl)amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



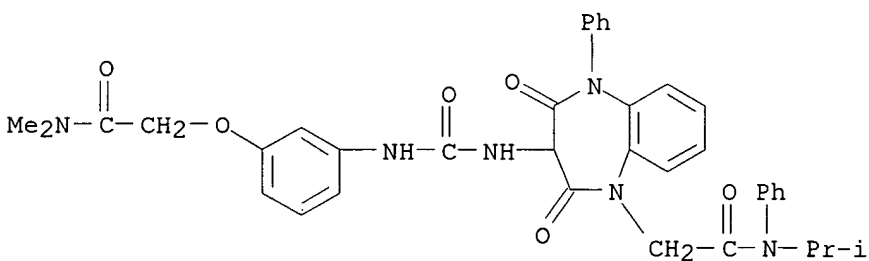
RN 184945-12-8 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[3-(2-amino-2-oxoethoxy)phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



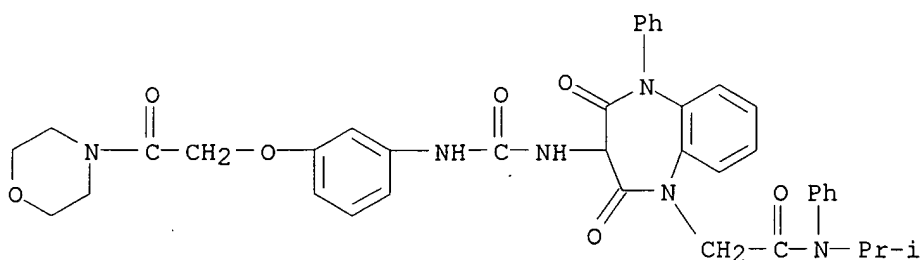
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CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[3-[2-(dimethylamino)-2-oxoethoxy]phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



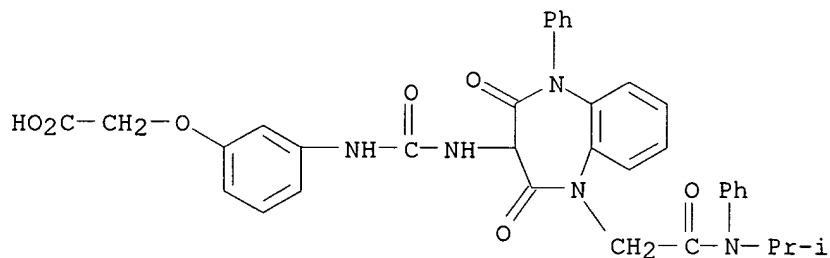
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CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[3-[2-(4-morpholinyl)-2-oxoethoxy]phenyl]amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



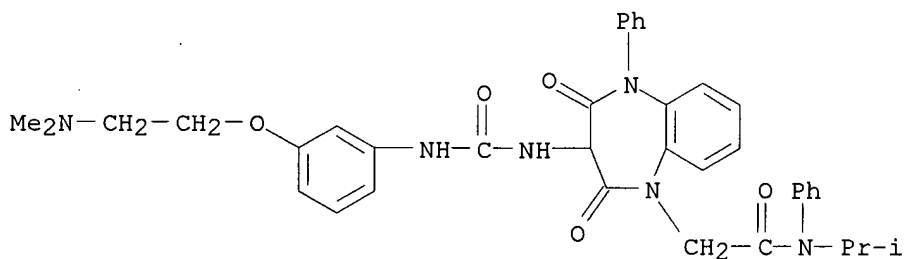
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CN Acetic acid, [3-[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]phenoxy]- (9CI) (CA INDEX NAME)



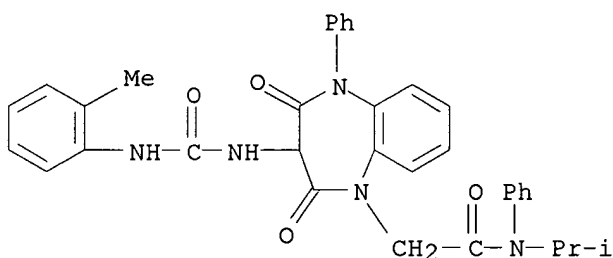
RN 184945-16-2 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[3-[2-(dimethylamino)ethoxy]phenyl]amino]carbonyl]amino]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



RN 184945-30-0 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[2-(2-methylphenyl)amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



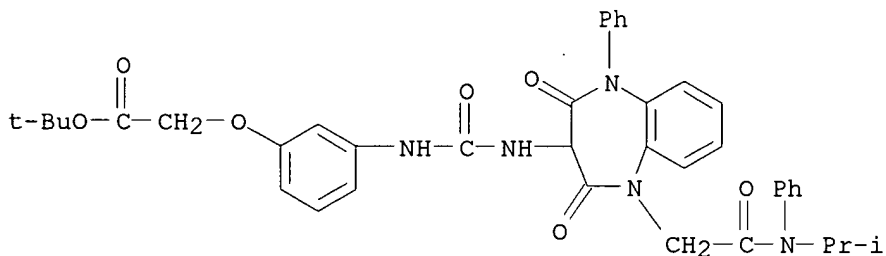
IT 184944-89-6P 184945-28-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and structure activity relations of 1,5-benzodiazepines as peripheral cholecystokinin (CCK-A) receptor agonists)

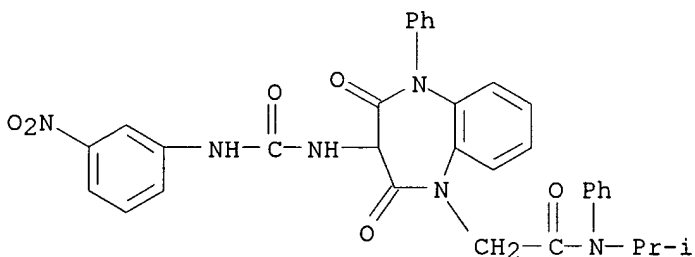
RN 184944-89-6 CAPLUS

CN Acetic acid, [3-[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]phenoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



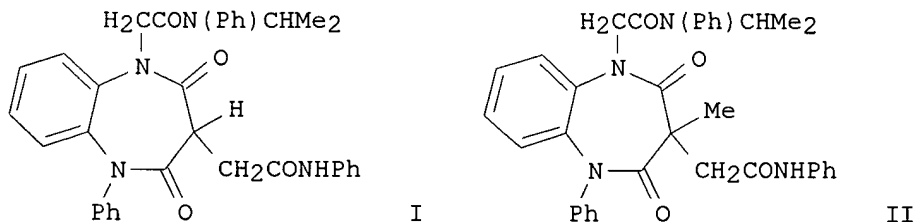
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CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-3-[[[3-nitrophenyl]amino]carbonyl]amino]-2,4-dioxo-N,5-diphenyl- (9CI) (CA INDEX NAME)



09/980,987

~~LI~~ ANSWER 7 OF 9 CAPLUS COPYRIGHT 2003 ACS
AN 1996:382879 CAPLUS
DN 125:104231
TI 3-[2-(N-Phenylacetamide)]-1,5-benzodiazepines: Orally Active, Binding
Selective CCK-A Agonists
AU Willson, Timothy M.; Henke, Brad R.; Momtahan, Tanya M.; Myers, Peter L.;
Sugg, Elizabeth E.; Unwalla, Rayomand J.; Croom, Dallas K.; Dougherty,
Robert W.; Grizzle, Mary K.; et al.
CS Glaxo Wellcome Research and Development, Research Triangle Park, NC,
27709, USA
SO Journal of Medicinal Chemistry (1996), 39(15), 3030-3034
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI

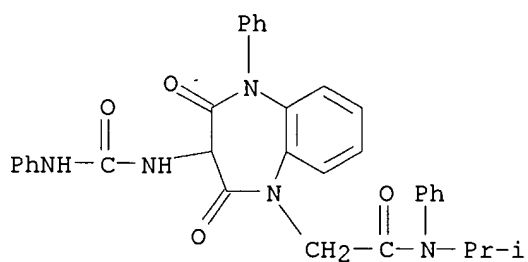


AB A series of modifications were made to the C-3 substituent of the
1,5-benzodiazepine CCK-A agonist I. Replacement of the inner urea NH and
addn. of a Me group to generate a C-3 quaternary carbon resulted in
acetamide II, which showed CCK-A receptor binding selectivity and
sub-micromolar agonist activity in vitro. II was active in an in vivo
mouse gallbladder emptying assay and represents a novel orally active,
binding selective CCK-A agonist.

IT **173908-75-3P 178983-16-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(prepn. of 3-[2-(N-phenylacetamide)]-1,5-benzodiazepines as orally
active, binding selective CCK-A agonists)

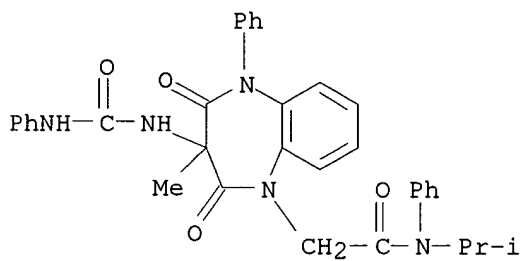
RN 173908-75-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-
2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX
NAME)

09/980,987

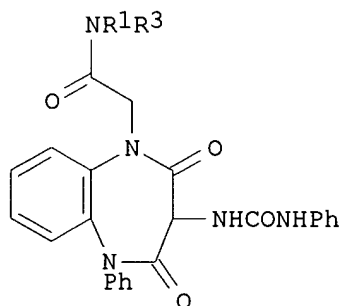


RN 178983-16-9 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-methyl-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



~~17~~ ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS
 AN 1996:6885 CAPLUS
 DN 124:176049
 TI Discovery of 1,5-benzodiazepines with peripheral cholecystokinin (CCK-A) receptor agonist activity. 1. Optimization of the agonist "trigger"
 AU Aquino, Christopher J.; Armour, Duncan R.; Berman, Judd M.; Birkemo, Larry S.; Carr, Robin A. E.; Croom, Dallas K.; Dezube, Milana; Dougherty, Robert W., Jr.; Ervin, Gregory N.; et al.
 CS Department of Medicinal Chemistry, Glaxo Wellcome, Research Triangle Park, NC, 27709, USA
 SO Journal of Medicinal Chemistry (1996), 39(2), 562-9
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 GI



AB Directed screening of compds. selected from the Glaxo registry file for contractile activity on the isolated guinea pig gallbladder identified a series of 1,5-benzodiazepines [I; R1 = H, Me, Et, Pr, Bu, CH2CH2CN, CHMe2, cyclohexyl, Ph, etc.; R3 = (substituted) Ph, etc.] with peripheral cholecystokinin (CCK) receptor agonist activity. Agonist efficacy within this series was modulated by variation of substituents on the N1-anilinoacetamide moiety. Remarkably, a single Me group confers agonist activity, with a CHMe2 providing optimal efficacy. Hydrophilic substituents on the anilino N abolish agonist activity or produce antagonists of CCK. In contrast, hydrophilic electron-donating groups at the para-position of the anilino ring enhance or maintain in vitro and in vivo agonist activity. Despite decreased affinity for the human CCK-A receptor relative to CCK-8, some I are equipotent to CCK as anorectic agents in rats following i.p. administration.

IT 173908-65-1P 173908-66-2P 173908-67-3P
 173908-68-4P 173908-69-5P 173908-70-8P
 173908-71-9P 173908-72-0P 173908-73-1P
 173908-74-2P 173908-75-3P 173908-76-4P
 173908-77-5P 173908-78-6P 173908-79-7P
 173908-81-1P 173908-82-2P 173908-83-3P
 173908-84-4P 173908-85-5P 173908-86-6P
 173908-87-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

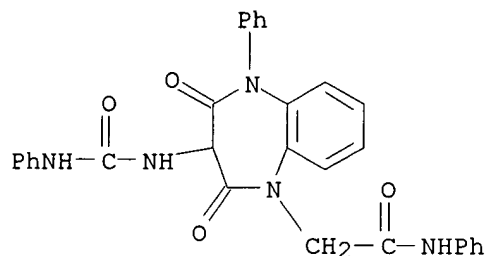
(prepn. of 1,5-benzodiazepines with peripheral cholecystokinin (CCK-A))

09/980,987

agonist activity)

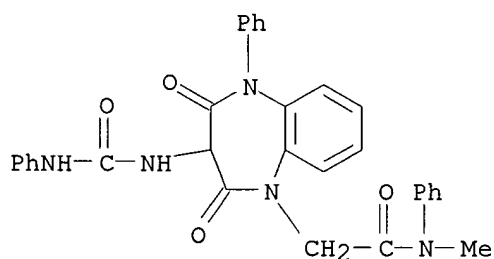
RN 173908-65-1 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



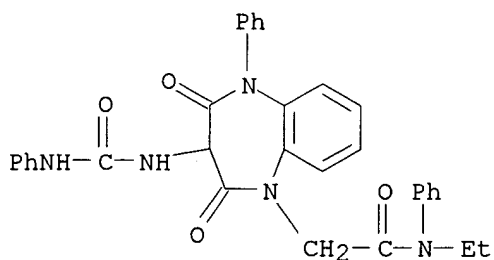
RN 173908-66-2 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-methyl-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



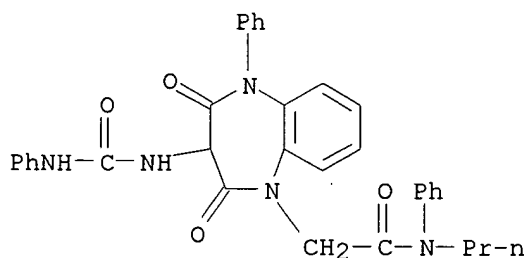
RN 173908-67-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-ethyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



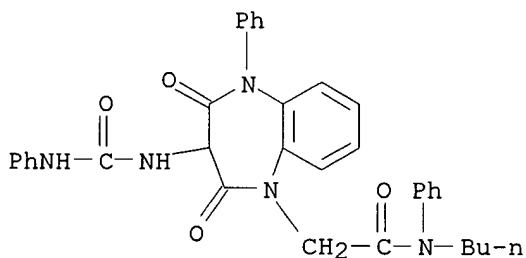
RN 173908-68-4 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]-N-propyl- (9CI) (CA INDEX NAME)



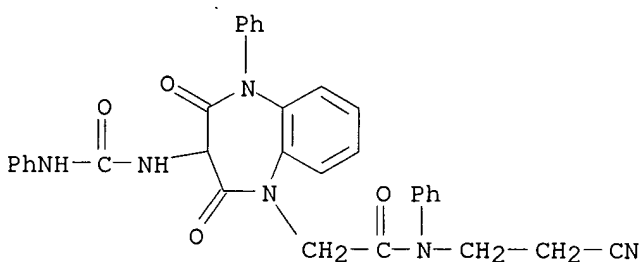
RN 173908-69-5 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-butyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



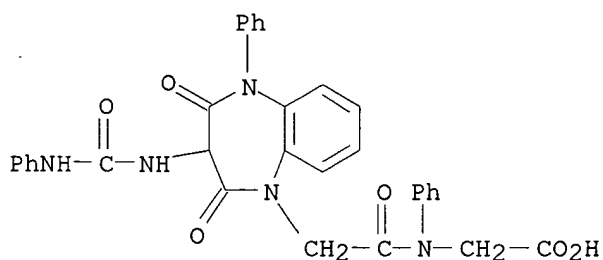
RN 173908-70-8 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-cyanoethyl)-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)

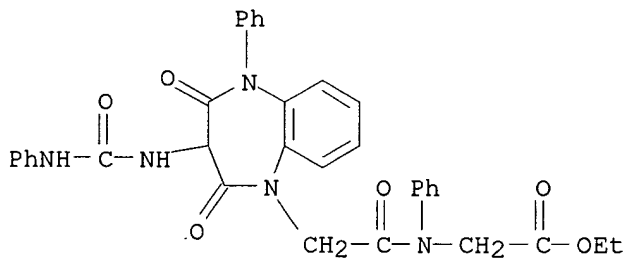


RN 173908-71-9 CAPLUS

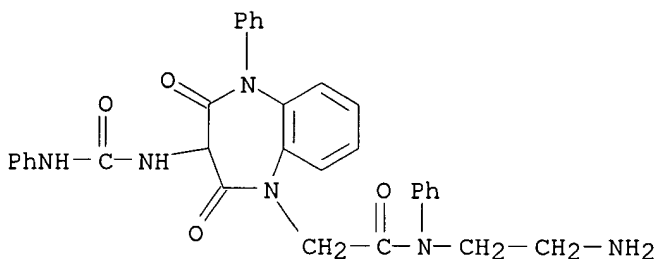
CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)



RN 173908-72-0 CAPLUS

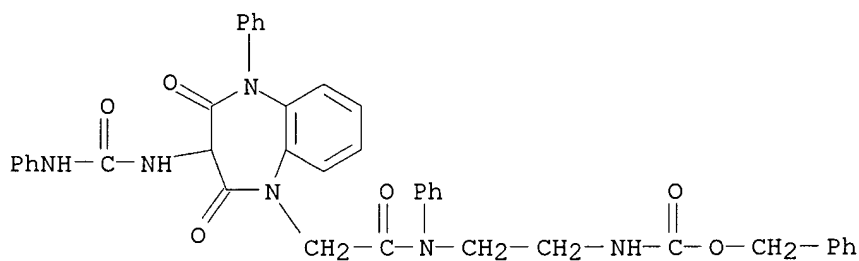
CN Glycine, N-phenyl-N-[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-
[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-yl]acetyl]-, ethyl
ester (9CI) (CA INDEX NAME)

RN 173908-73-1 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-(2-aminoethyl)-2,3,4,5-tetrahydro-2,4-
dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX
NAME)

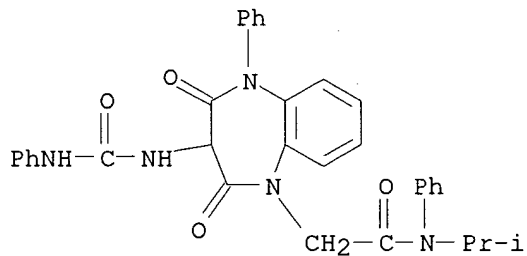
RN 173908-74-2 CAPLUS

CN Carbamic acid, [2-[phenyl[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-
[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-
yl]acetyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



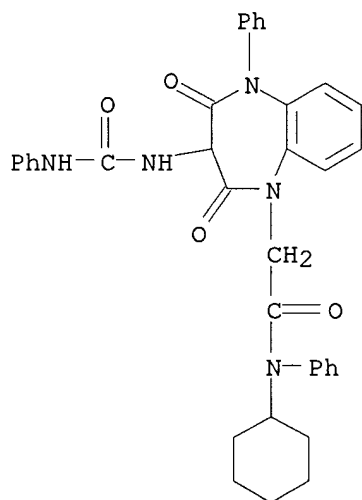
RN 173908-75-3 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[(phenylamino)carbonyl]amino- (9CI) (CA INDEX NAME)



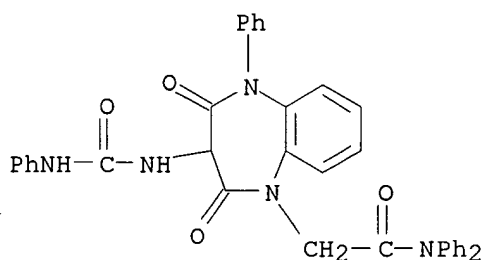
RN 173908-76-4 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-cyclohexyl-2,3,4,5-tetrahydro-2,4-dioxo-N,5-diphenyl-3-[(phenylamino)carbonyl]amino- (9CI) (CA INDEX NAME)



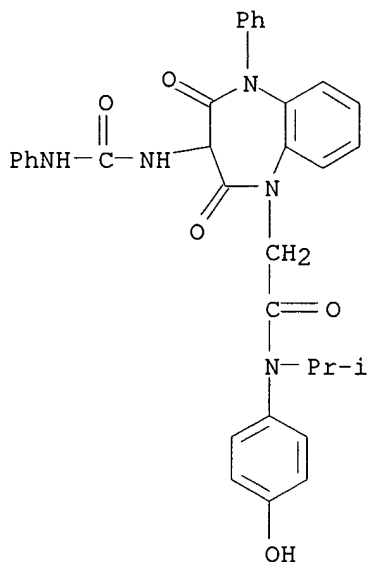
RN 173908-77-5 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-2,4-dioxo-N,N,5-triphenyl-3-[(phenylamino)carbonyl]amino- (9CI) (CA INDEX NAME)



RN 173908-78-6 CAPLUS

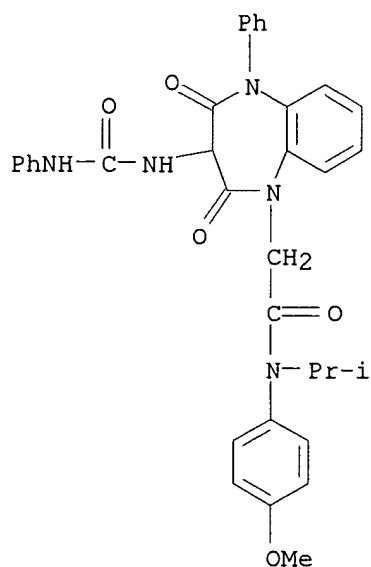
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-hydroxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



RN 173908-79-7 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(4-methoxyphenyl)-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)

09/980,987



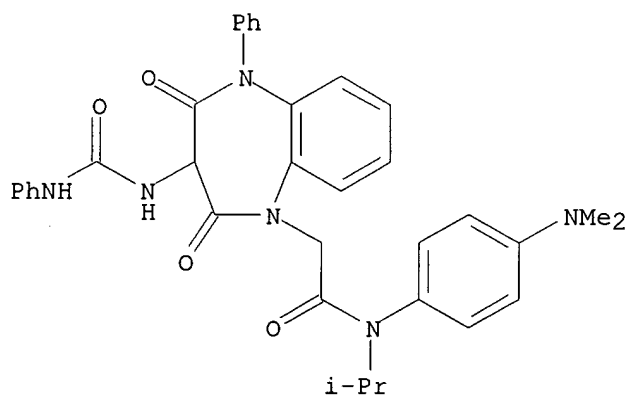
RN 173908-81-1 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 161456-17-3

CMF C35 H36 N6 O4

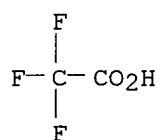


CM 2

CRN 76-05-1

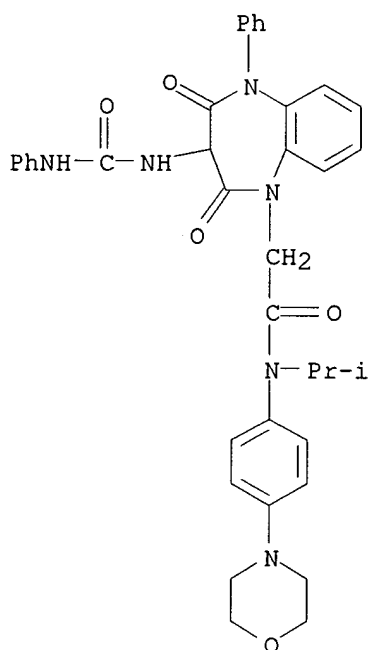
CMF C2 H F3 O2

09/980,987



RN 173908-82-2 CAPLUS

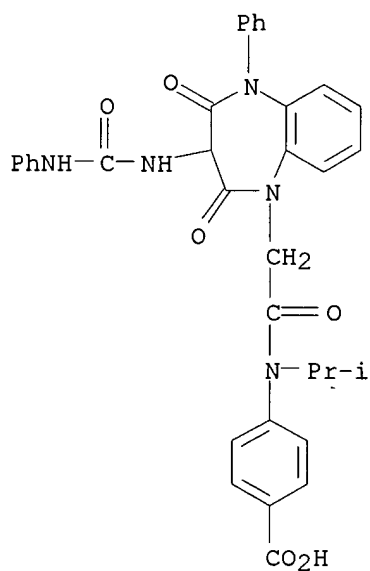
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-N-[4-(4-morpholinyl)phenyl]-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino] - (9CI) (CA INDEX NAME)



RN 173908-83-3 CAPLUS

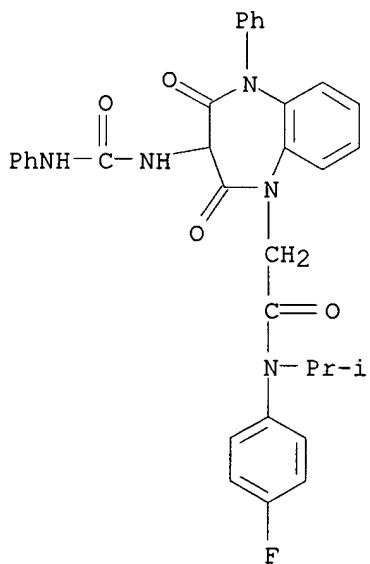
CN Benzoic acid, 4-[(1-methylethyl)[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-yl]acetyl] amino] - (9CI) (CA INDEX NAME)

09/980,987



RN 173908-84-4 CAPLUS

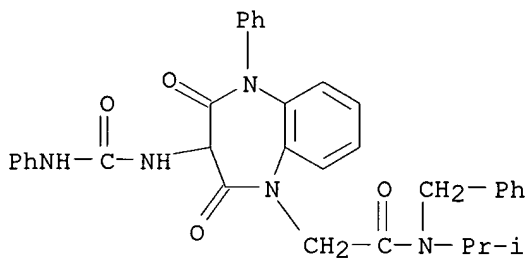
CN 1H-1,5-Benzodiazepine-1-acetamide, N-(4-fluorophenyl)-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[(phenylamino)carbonyl]amino- (9CI)
(CA INDEX NAME)



RN 173908-85-5 CAPLUS

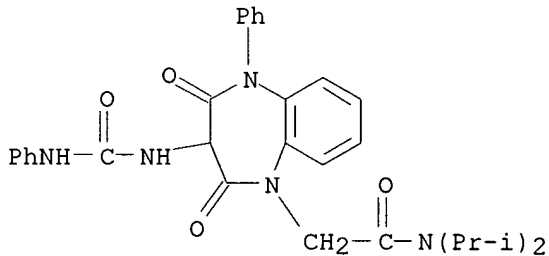
CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[(phenylamino)carbonyl]amino-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

09/980,987



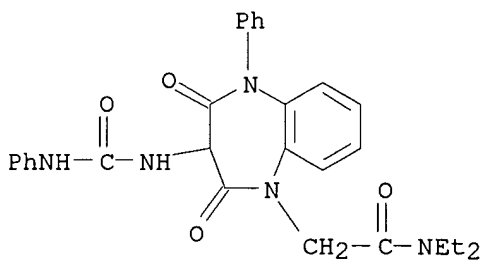
RN 173908-86-6 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N,N-bis(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]- (9CI)
(CA INDEX NAME)



RN 173908-87-7 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, N,N-diethyl-2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



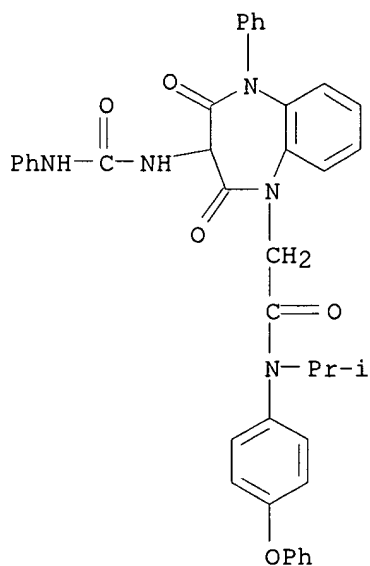
IT **173908-92-4 173908-93-5**

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of 1,5-benzodiazepines with peripheral cholecystokinin (CCK-A) agonist activity)

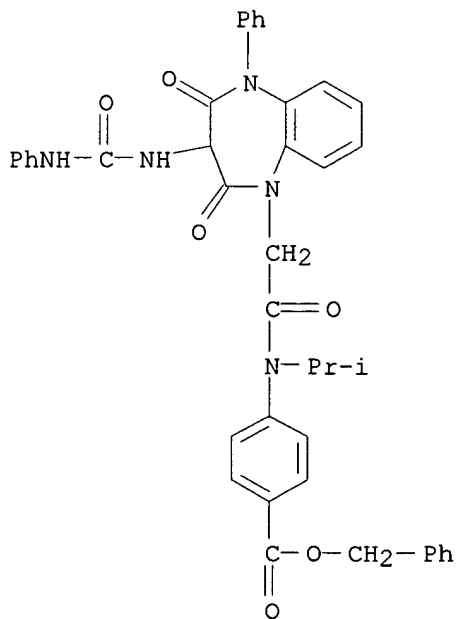
RN 173908-92-4 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N-(4-phenoxyphenyl)-5-phenyl-3-[[(phenylamino) carbonyl] amino]- (9CI) (CA INDEX NAME)



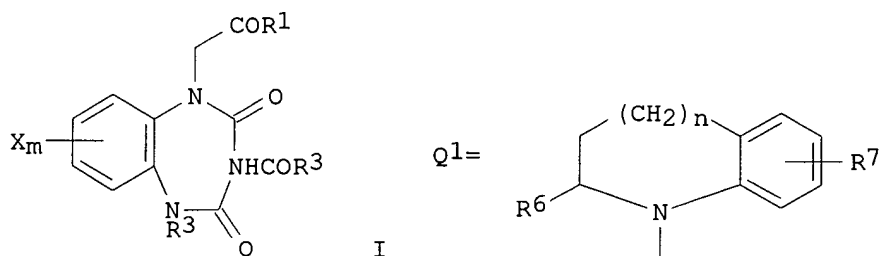
RN 173908-93-5 CAPLUS

CN Benzoic acid, 4-[(1-methylethyl)[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino) carbonyl] amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS
 AN 1995:408461 CAPLUS
 DN 122:187628
 TI Preparation of 1,5-benzodiazepine-2,4-dione derivatives as cholecystokinin
 A receptor agonists.
 IN Sugg, Elizabeth Ellen; Aquino, Christopher Joseph; Szewczyk, Jerzy
 Ryszard; Finch, Harry; Carr, Robin Arthur Ellis
 PA Glaxo Inc., USA
 SO PCT Int. Appl., 61 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9424149	A1	19941027	WO 1994-EP1131	19940414
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	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	IL 109316	A1	19990312	IL 1994-109316	19940413
	CA 2158973	AA	19941027	CA 1994-2158973	19940414
	AU 9465676	A1	19941108	AU 1994-65676	19940414
	AU 681139	B2	19970821		
	ZA 9402570	A	19941111	ZA 1994-2570	19940414
	ZA 9402571	A	19941111	ZA 1994-2571	19940414
	EP 694039	A1	19960131	EP 1994-913580	19940414
	EP 694039	B1	20010124		
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	RU 2135486	C1	19990827	RU 1995-117974	19940414
	CZ 286695	B6	20000614	CZ 1995-2675	19940414
	PL 178790	B1	20000630	PL 1994-311084	19940414
	SK 281211	B6	20010118	SK 1995-1253	19940414
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	ES 2154674	T3	20010416	ES 1994-913580	19940414
	FI 9504853	A	19951012	FI 1995-4853	19951012
	NO 9504090	A	19951213	NO 1995-4090	19951013
	US 5646140	A	19970708	US 1995-525659	19951013
PRAI	GB 1993-7833	A	19930415		
	WO 1994-EP1131	W	19940414		
OS	MARPAT 122:187628				
GI					



AB Title compds. [I; X = H, CF₃, alkyl, alkylthio, alkoxy, halo; R₁ = amino, Q₁; R₂ = (substituted) pyrrolyl, quinoliny, benzofuryl, benzothieryl, indolyl, indoliny, Ph, pyridyl, amino, etc.; R₃ = H, alkyl, cycloalkyl, (halo)phenyl; R₆ = H, Me; R₇ = H, OH, F, Me₂N, alkoxy, PhCH₂O; m, n = 1, 2], were prepd. Thus, 2-(3-amino-2,4-dioxo-5-phenyl-2,3,4,5-tetrahydrobenzo[b][1,4]diazepin-1-yl)-N-isopropyl-N-(4-methoxyphenyl)acetamide (prepn. given) was stirred with indole-2-carboxylic acid, hydroxybenzotriazole, and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride in DMF to give 1H-indole-2-carboxylic acid [1-[1-isopropyl-(4-methoxyphenyl)carbamoylmethyl]-2,4-dioxo-5-phenyl-2,3,4,5-tetrahydro-1H-benzo[b][1,4]diazepin-3-yl]amide. The latter at 30 .mu.M in a guinea pig gall bladder assay gave 42% contraction relative to acetylcholine at 100%.

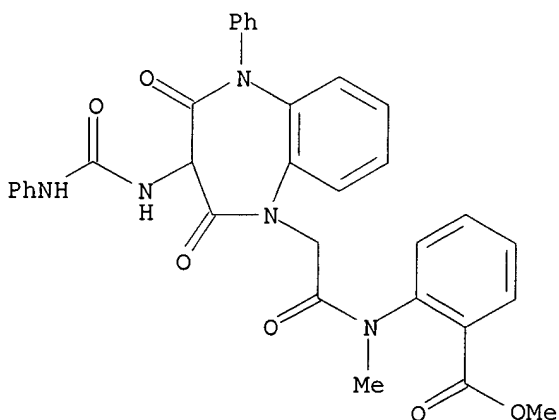
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 161456-15-1 161456-16-2 161456-17-3
 161456-18-4 161456-19-5 161456-20-8
 161456-30-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(1,5-benzodiazepine derivs. as cholecystokinin A agonists)

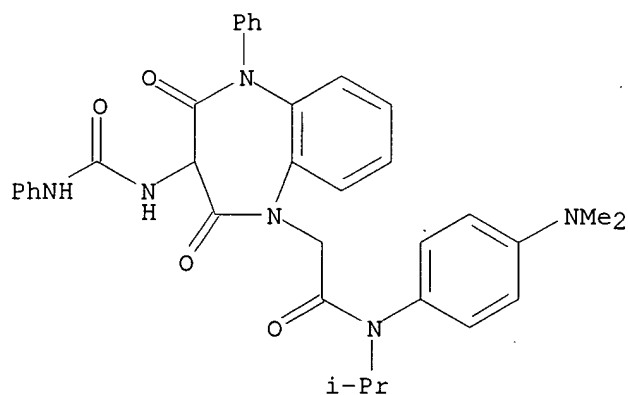
RN 161455-99-8 CAPLUS

CN Benzoic acid, 2-[methyl[[2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]-1H-1,5-benzodiazepin-1-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

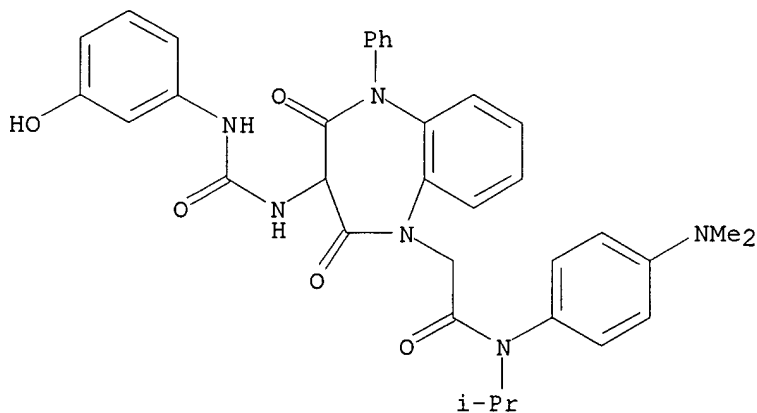


09/980,987

RN 161456-00-4 CAPLUS
RN 161456-01-5 CAPLUS
RN 161456-02-6 CAPLUS
RN 161456-13-9 CAPLUS
RN 161456-14-0 CAPLUS
RN 161456-15-1 CAPLUS
RN 161456-16-2 CAPLUS
RN 161456-17-3 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl-3-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)

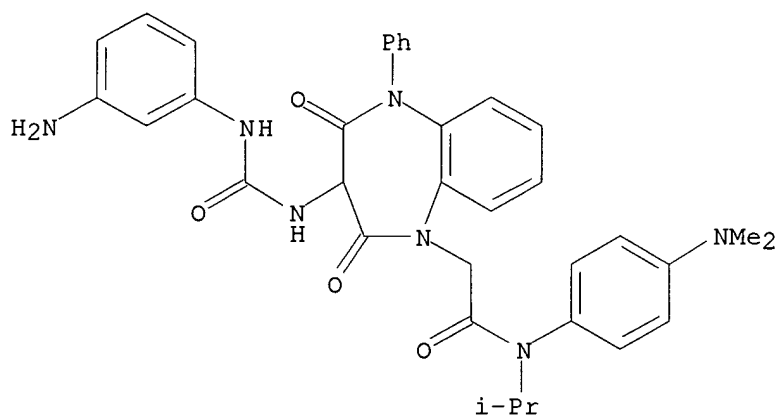


RN 161456-18-4 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-3-[[[(3-hydroxyphenyl) amino] carbonyl] amino]-N-(1-methylethyl)-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



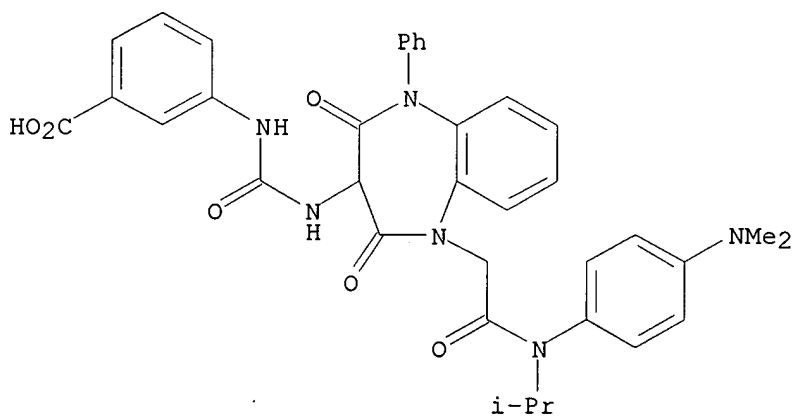
RN 161456-19-5 CAPLUS
CN 1H-1,5-Benzodiazepine-1-acetamide, 3-[[[(3-aminophenyl) amino] carbonyl] amino]-N-[4-(dimethylamino)phenyl]-2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)

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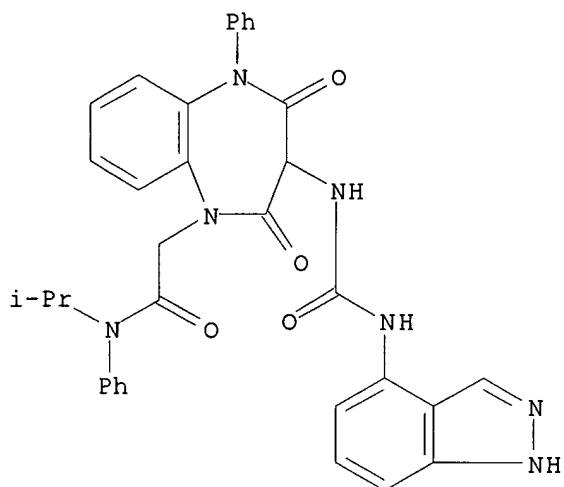
RN 161456-20-8 CAPLUS

CN Benzoic acid, 3-[[[1-[2-[[4-(dimethylamino)phenyl](1-methylethyl)amino]-2-oxoethyl]-2,3,4,5-tetrahydro-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 161456-30-0 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-3-[[[(1H-indazol-4-ylamino)carbonyl]amino]-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl]- (9CI) (CA INDEX NAME)



IT 161455-77-2P 161455-81-8P 161455-82-9P
161455-83-0P 161513-73-1P 161513-74-2P

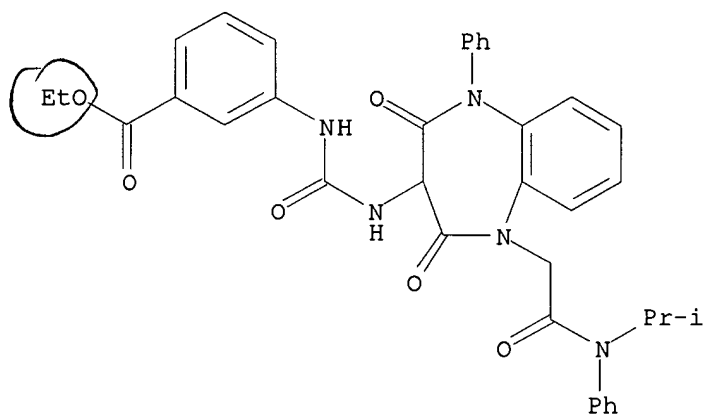
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 1,5-benzodiazepine derivs. as cholecystokinin A agonists)

RN 161455-77-2 CAPLUS

RN 161455-81-8 CAPLUS

RN 161455-82-9 CAPLUS

CN Benzoic acid, 3-[[[2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1H-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



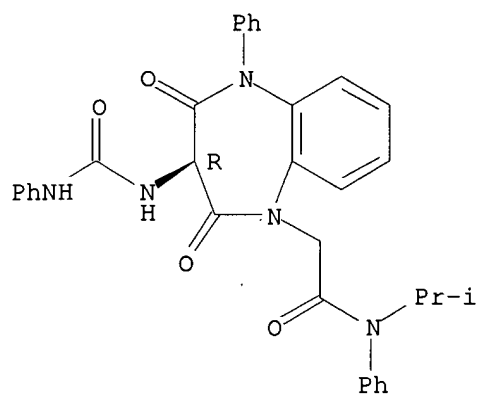
RN 161455-83-0 CAPLUS

RN 161513-73-1 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-2,4-dioxo-N,5-diphenyl-3-[[[(phenylamino)carbonyl]amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 161513-74-2 CAPLUS

CN 1H-1,5-Benzodiazepine-1-acetamide, 2,3,4,5-tetrahydro-N-(1-methylethyl)-
2,4-dioxo-N,5-diphenyl-3-[[(phenylamino) carbonyl] amino]-, (S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

